

Technical Note: Proximal Ordered Subsets Algorithms for TV Constrained Optimization in CT Image Reconstruction

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Abstract

This article is intended to supplement our recent paper [S. Rose et al., “Noise properties of CT images reconstructed by use of constrained total-variation, data-discrepancy minimization,” *Med. Phys.*, vol. 42, pp. 2690–2698, 2015] in which ordered subsets methods were employed to perform total-variation (TV) constrained data-discrepancy minimization for image reconstruction in X-ray computed tomography (CT). Here we provide details regarding implementation of the ordered subsets algorithms and suggestions for selection of algorithm parameters. Detailed pseudo-code is included for every algorithm implemented in the original manuscript.

I. INTRODUCTION

In our recent paper on the noise properties of images reconstructed using total-variation (TV) constrained data-discrepancy minimization [1], ordered subsets methods — also referred to as incremental, row-action, and batch methods — were employed to perform constrained optimization. This was motivated in part by recent work in the optimization community in which the convergence properties of a general class of proximal-gradient ordered subsets algorithms were investigated [2, 3]. Here, detailed instructions and pseudo-code are provided for implementing ordered subsets algorithms for total-variation constrained weighted least squares (TVC-WLSQ) and Poisson likelihood (TVC-PL) optimization in computed tomographic (CT) image reconstruction. In section II the design of the ordered subsets algorithms is outlined following the framework developed in [2]. In section III it is demonstrated how one can perform projection onto a TV-ball using a first order primal dual algorithm proposed by Chambolle and Pock [4]. In section IV full pseudo-code is provided for each algorithm with some additional notes and recommendations for implementation.

II. ALGORITHM DESIGN

The proximal gradient ordered subsets framework applies to optimization problems in which the objective function can be separated into a sum of component functions as follows

$$\min_{x \in X} \sum_{i=1}^S (g_i(x) + h_i(x)) \quad (\text{P1})$$

where $g_i, h_i : \mathbb{R}^n \mapsto \mathbb{R}$ are convex functions and X is a convex set. Ordered subsets algorithms operate on individual component functions one at a time instead of utilizing the entire objective function for every

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update. The ordered subsets algorithm used in our recent paper, and originally proposed in [2], has the form

$$\begin{aligned} q^k &= \text{prox}_{t_k g_{i_k}}(x^k) \\ x^{k+1} &= \mathcal{P}(q^k - t_k \tilde{\nabla} h_{i_k}(q^k); X) \end{aligned} \quad (1)$$

where $\mathcal{P}(\cdot; X)$ represents projection onto X , $\tilde{\nabla} h(q)$ represents a subgradient of h at q , and the proximal operator is defined as

$$\text{prox}_f(x) = \underset{u}{\operatorname{argmin}} \left\{ f(u) + \frac{1}{2} \|u - x\|_2^2 \right\}$$

Here and throughout this document superscripts on vector quantities denote iterates of an algorithm, while superscripts attached to scalars denote raising the scalar to the given power. The value of i_k can be chosen in a cyclic fashion ($i_k = k \bmod S$) or in a randomized manner.

In this section, we derive ordered subsets algorithms for the TVC-WLSQ and TVC-PL reconstruction optimization problems using the update step in 1.

A. TVC-WLSQ

The TVC-WLSQ reconstruction optimization problem takes the form

$$\begin{aligned} \min_x \quad & \frac{1}{2} (Ax - b)^T \operatorname{diag}(w) (Ax - b) \\ \text{such that} \quad & \operatorname{TV}(x) \leq \gamma \end{aligned} \quad (\text{P2})$$

where $A \in \mathbb{R}^{m \times n}$ is the system matrix representing the forward model, $b \in \mathbb{R}^m$ is the measured sinogram data, $x \in \mathbb{R}^n$ is an image estimate, and $w \in \mathbb{R}_{++}^m$ is a strictly positive weighting vector. An ordered subsets algorithm can be derived by defining

$$\begin{aligned} g_i(x) &= \frac{1}{2} w_i (a_i^T x - b_i)^2 \text{ for } i = 1, \dots, m \\ h_i(x) &= 0 \text{ for } i = 1, \dots, m+1 \end{aligned}$$

and

$$g_{m+1}(x) = \delta(x; B_{\operatorname{TV}}(\gamma))$$

where

$$\delta(x; X) = \begin{cases} 0 & \text{if } x \in X \\ \infty & \text{else} \end{cases}$$

and $B_{\operatorname{TV}}(\gamma) = \{x : \operatorname{TV}(x) \leq \gamma\}$ is the TV ball of radius γ . The i^{th} row of the system matrix A has been denoted a_i^T . Note that in the definition of g_{m+1} the constraint has been imposed using an indicator function and X can therefore be taken to be \mathbb{R}^n .

It can be shown that [1]

$$\begin{aligned} \text{prox}_{t_k g_{i_k}}(x) &= x - \frac{a_{i_k}^T x - b_{i_k}}{(w_{i_k} t_k)^{-1} + \|a_{i_k}\|_2^2} a_{i_k} \text{ for } i_k = 1, \dots, m \\ \text{prox}_{t_k g_{m+1}}(x) &= \mathcal{P}(x, B_{\operatorname{TV}}(\gamma)) \end{aligned}$$

This yields the following algorithm

Algorithm 1 Ordered Subsets TVC-WLSQ

```
1: Initialize  $x_0$  to zero
2: for  $k = 0, \dots, K - 1$  do
3:    $p^0 \leftarrow x^k$ 
4:   for  $i = 0, \dots, m - 1$  do
5:      $p^{i+1} \leftarrow p^i - \frac{a_i^T p^i - b_i}{\|a_i\|_2^2 + (t_k w_i)^{-1}} a_i$ 
6:   end for
7:    $x^{k+1} \leftarrow \mathcal{P}(p^m, B_{\text{TV}}(\gamma))$ 
8: end for
```

The sub-iterations for p are similar in nature to the algebraic reconstruction technique (ART) [5], involving a loop over the data with an image update based upon each ray. Note that by imposing the TV constraint as an indicator function one obtains an algorithm which involves projection onto the constraint set only once per loop over the data. The projection onto the TV-ball must be done using a numerical method. In section III, it is shown how to perform this operation with the primal-dual algorithm of Chambolle and Pock (CP algorithm) [4].

The choice of step-size t_k can have a significant effect on convergence rate. To ensure convergence, a diminishing step-size is required. We have found the following step-size rule to be useful in practice

$$c_k = \left\lfloor \frac{k}{r} \right\rfloor + 1$$
$$t_k = \frac{1}{c_k}$$

where r represents the number of steps for which we hold the step-size constant and $\lfloor \cdot \rfloor$ denotes the floor operation. In our studies, r is often taken to be 20, but we suggest experimentation to determine a reasonable value for any given scenario.

B. TVC-PL

The reconstruction optimization problem for TVC-PL is given by

$$\min_x \sum_{i=1}^m (y_i a_i^T x + N_0 \exp(-a_i^T x)) \tag{P3}$$

such that $\text{TV}(x) \leq \gamma$

where $y \in \mathbb{R}^m$ is the measured transmission data and N_0 is the number of incident photons per ray. An incremental algorithm is derived from the update step in 1 using the following definitions

$$g_i(x) = y_i a_i^T x + N_0 \exp(-a_i^T x) \text{ for } i = 1, \dots, m$$
$$h_i(x) = 0 \text{ for } i = 1, \dots, m + 1$$

and

$$g_{m+1}(x) = \delta(x; B_{\text{TV}}(\gamma))$$

It can be shown that [1]

$$\text{prox}_{t_k g_{i_k}}(x^k) = x^k + t_k(N_0 \exp(-c_k^*) - y_{i_k})a_{i_k} \text{ for } i_k = 1, \dots, m$$

where c_k^* is found by implicit solution of

$$c_k^* = a_{i_k}^T x + t_k \|a_{i_k}\|_2^2 (N_0 \exp(-c_k^*) - y_{i_k})$$

Methods for calculating c_k^* are provided in [1]. The proximal operation for g_{m+1} is the same as for TVC-WLSQ.

Plugging the derived proximal updates into 1 yields the following algorithm.

Algorithm 2 Ordered Subsets TVC-PL

```

1: Initialize  $x_0$  to zero
2: for  $k = 0, \dots, K - 1$  do
3:    $p^0 \leftarrow x^k$ 
4:   for  $i = 0, \dots, m - 1$  do
5:     Solve  $c_i^* = a_i^T p^i + t_k \|a_i\|_2^2 (N_0 \exp(-c_i^*) - y_i)$  for  $c_i^*$ 
6:      $p^{i+1} \leftarrow p^i + t_k (N_0 \exp(-c_i^*) - y_i) a_i$ 
7:   end for
8:    $x^{k+1} \leftarrow \mathcal{P}(p^m, B_{\text{TV}}(\gamma))$ 
9: end for

```

III. CHAMBOLLE-POCK ALGORITHM FOR PROJECTION ONTO TV BALL: DERIVATION AND PSEUDO-CODE

Here the derivation and pseudo-code of an instance of the CP algorithm are presented for projection of an image onto a TV-ball of radius γ . The derivation follows the framework and notation presented by Sidky et al. [6] in which the algorithm was applied to a variety of optimization problems for CT image reconstruction.

The Chambolle-Pock algorithm is used to solve convex optimization problems written in the form

$$\min_s F(Ks) + G(s)$$

Here the algorithm is employed to solve the problem of projecting onto $B_{\text{TV}}(\gamma)$, which can be expressed as

$$\begin{aligned} & \min_s \frac{1}{2} \|s - x\|_2^2 \\ & \text{such that } \|h(D_1 s, D_2 s)\|_1 \leq \gamma \end{aligned}$$

where $h : \mathbb{R}^{2n} \mapsto \mathbb{R}^n$ is defined by

$$h_i(y, z) = \sqrt{y_i^2 + z_i^2}$$

The operators $D_1 : \mathbb{R}^n \mapsto \mathbb{R}^n$ and $D_2 : \mathbb{R}^n \mapsto \mathbb{R}^n$ are finite difference operators which calculate approximations of the x and y components of the spatial gradients of the image, respectively.

For the purposes of applying the algorithm, define

$$\begin{aligned} F(y, z) &= \delta(h(y, z); B_1(\gamma)) \\ G(s) &= \frac{1}{2} \|s - x\|_2^2 \\ K &= \begin{pmatrix} D_1 \\ D_2 \end{pmatrix} \end{aligned}$$

where $B_1(\gamma) = \{s : \|s\|_1 \leq \gamma\}$.

In this section, pseudo-code is first presented for the instance of the CP algorithm these definitions yield. A detailed derivation of the proximal mappings used in the pseudo-code follows.

A. TV Projection Pseudo-code

The Chambolle Pock update for projection onto the TV ball takes the form

Algorithm 3 Projection onto TV ball

```

1:  $L \leftarrow \left\| \begin{pmatrix} D_1 \\ D_2 \end{pmatrix} \right\|_2$ ;  $\tau \leftarrow 1/L$ ;  $\sigma \leftarrow 1/L$ ;  $\theta \leftarrow 1$ ;  $k \leftarrow 0$ 
2: Initialize  $s_0$ ,  $y_0$ , and  $z_0$ 
3:  $\bar{s} \leftarrow s_0$ 
4: for  $k = 0, \dots, K - 1$  do
5:    $y^k \leftarrow y^k + \sigma D_1 \bar{s}^k$ 
6:    $z^k \leftarrow z^k + \sigma D_2 \bar{s}^k$ 
7:    $v \leftarrow \frac{\mathcal{P}(h(y^k, z^k)/\sigma; B_1(\gamma))}{h(y^k, z^k)}$ 
8:    $\begin{pmatrix} y^{k+1} \\ z^{k+1} \end{pmatrix} \leftarrow \begin{pmatrix} y^k \\ z^k \end{pmatrix} - \sigma \begin{pmatrix} \text{diag}(v) & 0 \\ 0 & \text{diag}(v) \end{pmatrix} \begin{pmatrix} y^k \\ z^k \end{pmatrix}$ 
9:    $s^{k+1} \leftarrow s^k - \tau (D_1^T, D_2^T) \begin{pmatrix} y^{k+1} \\ z^{k+1} \end{pmatrix}$ 
10:   $s^{k+1} \leftarrow \frac{s^{k+1}/\tau + b}{1 + 1/\tau}$ 
11:   $\bar{s}^{k+1} = s^{k+1} + \theta(s^{k+1} - s^k)$ 
12: end for
```

Calculating the ℓ_2 norm of a matrix — needed to calculate L — can be done with the power method [6]. In order to implement the projection algorithm, one must also be able to perform projection onto the ℓ_1 ball. This can be done using the method of Duchi et al. [7], which is presented as algorithm 2 in another of our recent papers [8]. In practice, the TV-projection algorithm is only run for approximately 10 iterations, yielding an inexact projection onto the TV-ball. It is important when running the algorithm to monitor the TV of the individual iterates to make sure the algorithm yields a result which is inside or close to the TV-ball.

B. Proximal Mapping of G

Here the proximal mapping of G

$$\text{prox}_{\tau G}(s) = \underset{u}{\operatorname{argmin}} \left\{ \frac{1}{2} \|u - x\|_2^2 + \frac{\|u - s\|_2^2}{2\tau} \right\}$$

is derived. The first order optimality conditions yield

$$\begin{aligned} (u^* - x) + \frac{1}{\tau}(u^* - s) &= 0 \\ \implies \left(1 + \frac{1}{\tau}\right)u^* &= x + s/\tau \\ \implies \text{prox}_{\tau G}(s) &= \frac{x + s/\tau}{1 + 1/\tau} \end{aligned}$$

C. Proximal Mapping of F^*

To find the proximal mapping of F^* , one can employ the Moreau identity

$$\text{prox}_{\sigma F^*}(y, z) = \begin{pmatrix} y \\ z \end{pmatrix} - \sigma \text{prox}_{F/\sigma}(y/\sigma, z/\sigma)$$

It is then necessary to evaluate

$$\text{prox}_F(y, z) = \underset{\substack{u, w \\ h(u, w) \in B_1(\gamma)}}{\text{argmin}} \{ \|u - y\|_2^2 + \|w - z\|_2^2 \}$$

To do so, note that the minimization can be separated component-wise. It can then be seen

$$\begin{aligned} (u_i - y_i)^2 + (w_i - z_i)^2 &= (u_i^2 + w_i^2) + (y_i^2 + z_i^2) - 2(u_i y_i + w_i z_i) \\ &\geq (u_i^2 + w_i^2) + (y_i^2 + z_i^2) - 2\|(u_i, w_i)^T\| \|(y_i, z_i)^T\| \\ &= (h_i(u, w) - h_i(y, z))^2 \end{aligned}$$

where the second line follows from the Cauchy-Schwarz inequality. Equality holds throughout if

$$(u_i, w_i)^T = c_i (y_i, z_i)^T, \quad i = 1, \dots, n; \quad c_i \geq 0$$

One can therefore evaluate the proximal mapping by first projecting $h(y, z)$ onto the ℓ_1 ball of radius γ yielding a vector $g^* \in \mathbb{R}^n$. One must then choose (u, w) such that $h(u, w) = g^*$ and $(u_i, w_i)^T = c_i (y_i, z_i)^T$. This can be done by scaling each vector (y_i, z_i) by the amount $c_i = g_i^* / \|(y_i, z_i)^T\|_2$ if $\|(y_i, z_i)^T\|_2 > 0$, and $c_i = 0$ otherwise. It follows that

$$\text{prox}_F(y, z) = \begin{pmatrix} \text{diag} \left[\frac{\mathcal{P}(h(y, z); B_1(\gamma))}{h(y, z)} \right] & 0 \\ 0 & \text{diag} \left[\frac{\mathcal{P}(h(y, z); B_1(\gamma))}{h(y, z)} \right] \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix}$$

where division of vectors is to be interpreted element-wise. Also note the slight abuse of notation in that the i^{th} element of $\frac{\mathcal{P}(h(y, z); B_1(\gamma))}{h(y, z)}$ should be 0 if $h_i(x, y)$ is 0. By substituting variables, one finds

$$\text{prox}_{F/\sigma}(y/\sigma, z/\sigma) = \begin{pmatrix} \text{diag} \left[\frac{\mathcal{P}(h(y/\sigma, z/\sigma); B_1(\gamma))}{h(y, z)} \right] & 0 \\ 0 & \text{diag} \left[\frac{\mathcal{P}(h(y/\sigma, z/\sigma); B_1(\gamma))}{h(y, z)} \right] \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix}$$

Plugging into the Moreau identity yields

$$\text{prox}_{\sigma F^*}(y, z) = \begin{pmatrix} y \\ z \end{pmatrix} - \sigma \begin{pmatrix} \text{diag} \left[\frac{\mathcal{P}(h(y/\sigma, z/\sigma); B_1(\gamma))}{h(y, z)} \right] & 0 \\ 0 & \text{diag} \left[\frac{\mathcal{P}(h(y/\sigma, z/\sigma); B_1(\gamma))}{h(y, z)} \right] \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix}$$

IV. THE FULL ALGORITHM

Here the full pseudo-code for the ordered subsets TVC-WLSQ and TVC-PL is presented. As noted previously, in our experience the parameter J , the number of iterations of the TV-projection algorithm, can typically be taken to be 10 and the step size chosen according to the rule

$$c_k = \left\lfloor \frac{k}{r} \right\rfloor + 1$$

$$t_k = \frac{1}{c_k}$$

with $r = 20$.

Algorithm 4 Ordered Subsets TVC-WLSQ

```

1:  $L \leftarrow \left\| \begin{pmatrix} D_1 \\ D_2 \end{pmatrix} \right\|_2$ ;  $\tau \leftarrow 1/L$ ;  $\sigma \leftarrow 1/L$ ;  $\theta \leftarrow 1$ ;  $k \leftarrow 0$ 
2: Initialize  $x^0, s^0, y^0$ , and  $z^0$  to zero ▷ Begin Iterating
3: for  $k = 0, \dots, K-1$  do
4:   Update step size  $t_k$ 
5:    $p^0 \leftarrow x^k$ 
6:   for  $i = 0, \dots, m-1$  do ▷ Run Incremental Update
7:      $p^{i+1} \leftarrow p^i - \frac{a_i^T p^i - b_i}{\|a_i\|_2^2 + (t_k w_i)^{-1}} a_i$ 
8:   end for
9:    $x^{k+1} \leftarrow p^m$ 
10:  if  $\text{TV}(x^{k+1}) > \gamma$  then ▷ Check TV
11:     $\bar{s}^0 \leftarrow s^0$ 
12:    for  $j = 0, \dots, J-1$  do ▷ Run Projection onto TV Ball
13:       $y^j \leftarrow y^j + \sigma D_1 \bar{s}^j$ 
14:       $z^j \leftarrow z^j + \sigma D_2 \bar{s}^j$ 
15:       $v \leftarrow \frac{\mathcal{P}(h(y^j/\sigma, z^j/\sigma); B_1(\gamma))}{h(y^j, z^j)}$ 
16:       $\begin{pmatrix} y^{j+1} \\ z^{j+1} \end{pmatrix} \leftarrow \begin{pmatrix} y^j \\ z^j \end{pmatrix} - \sigma \begin{pmatrix} \text{diag}(v) & 0 \\ 0 & \text{diag}(v) \end{pmatrix} \begin{pmatrix} y^j \\ z^j \end{pmatrix}$ 
17:       $s^{j+1} \leftarrow s^j - \tau (D_1^T, D_2^T) \begin{pmatrix} y^{j+1} \\ z^{j+1} \end{pmatrix}$ 
18:       $s^{j+1} \leftarrow \frac{s^{j+1}/\tau + x^{k+1}}{1 + 1/\tau}$ 
19:       $\bar{s}^{j+1} = s^{j+1} + \theta(s^{j+1} - s^j)$ 
20:    end for
21:     $x^{k+1} \leftarrow s^J$ 
22:     $s^0 \leftarrow s^J$  ▷ Save Variables for Warm Start
23:     $y^0 \leftarrow y^J$ 
24:     $z^0 \leftarrow z^J$ 
25:  end if
26: end for

```

As shown above, a warm start is used for the projection algorithm, by which it is meant that the last iterates of the s , y , and z variables are used to initialize s_0 , y_0 , and z_0 the next time projection needs

to be performed. Since the CP algorithm for projection onto the TV ball is truncated at early iteration, it is imperative that one monitors the TV of the iterates of the projection algorithm to ensure that it is performing correctly and that it outputs vectors which are close to or within the constraint set. The corresponding algorithm for TVC-PL is identical except for line 7, which must be replaced by lines 5 and 6 in Algorithm 2.

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